

Orthoformic acid, cyclic 2,2-dimethyltrimethylene ethyl ester
5783-79-9 | DTXSID20206542

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.40e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.84e-01

Confidence level: 5.81e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Phosmet</div> <div>Measured: 2.30e-02</div> <div>Predicted: 5.53e-07</div>	<div>Image not found</div> <div>Isopropyl octadecanoate</div> <div>Measured: 5.20e-01</div> <div>Predicted: 1.13e-05</div>	<div>Image not found</div> <div>Bis(2-chloroethoxy)methane</div> <div>Measured: 2.96</div> <div>Predicted: 1.91e-01</div>
<div>Image not found</div> <div>2-Undecanone</div> <div>Measured: 9.89e-02</div> <div>Predicted: 6.59e-02</div>	<div>Image not found</div> <div>1-Bromotetradecane</div> <div>Measured: 2.61e-02</div> <div>Predicted: 5.80e-04</div>	